

Mesh Independence of the Generalized Davidson Algorithm

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Abstract

We give conditions under which the generalized Davidson algorithm for eigenvalue computations is mesh-independent. In this case mesh-independence means that the iteration statistics (residual norms, convergence rates, for example) of a sequence of discretizations of a problem in a Banach space converge the statistics for the infinite-dimensional problem. We illustrate the result with several numerical examples.

Keywords: Generalized Davidson Algorithm; Mesh Independence; Neutron Transport; Electronic Structure Computations

1. Introduction

The purpose of this paper is to give conditions under which the residual norms of the generalized Davidson algorithm when applied to a finite-dimensional problem which approximates a problem in an infinite-dimensional space, converge to the residual norms of the Davidson iteration for the infinite dimensional problem. This is called mesh-independence in the nonlinear solver community [Allgower et al., 1986, Allgower and Böhm, 1987, Xue, 1995, Kelley and Sachs, 1991, 1992, Ferng and Kelley, 2000]. The idea is that one has an algorithm that makes some measure of error, such as the norm of a residual or a gradient, small. One applies this algorithm to a sequence of problems indexed with a parameter h , where h is, for example, a mesh-width, and observes that, for a given $\epsilon > 0$, the number of iterations needed to make the measure of error $< \epsilon$ is independent of h .

We will use the algorithmic descriptions from [Hamilton, 2011, Sleijpen and van der Vorst, 2000]. In the classic Davidson algorithm the preconditioner is the inverse of the diagonal of $\mathbf{A} - \lambda \mathbf{I}$. The generalized Davidson algorithm allows for any preconditioner $\mathbf{M} \approx \mathbf{A} - \lambda \mathbf{I}$. For simplicity we express Algorithm 1 as one designed to compute the smallest eigenvalue of $\mathbf{A}$, an operator in a finite or infinite dimensional Hilbert space with scalar product $(\cdot, \cdot)$ and norm $\|\cdot\|$. In the case where $\mathbf{A}$ is only densely defined then the inverse of the preconditioner must map residuals to the domain of $\mathbf{A}$.

The generalized Davidson algorithm is given by Algorithm 1.

In Algorithm 1 and for the rest of the paper we use bold faced fonts for vectors and operators which are finite dimensional or generic vectors and operators which can be either finite or infinite dimensional. We will use standard fonts for operators and vectors which are only defined in infinite dimensional spaces.

We will work in the following framework. We consider a possibly unbounded operator A defined on an infinite dimensional Hilbert space H . We let the domain of A be a Banach space X and the range Y . We let H denote the Hilbert space in which the orthogonalization in the generalized Davidson algorithm takes place, $(\cdot, \cdot)_H$ the inner product, and $\|u\|_H^2 = (u, u)_H$ for $u \in H$. Typically X is dense in H and the operator A is unbounded. We require $X \subset Y \subset H$.

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Algorithm 1 Generalized Davidson Algorithm

```
(u,  $\lambda$ ) = davidson(u0, A, M,  $\tau$ )
   $k = 0$ 
  v0 = u0 /  $\|\mathbf{u}_0\|$ 
  V0 = Span(v0)
   $\lambda_0 = (\mathbf{v}_0, \mathbf{A}\mathbf{v}_0)$ 
  r0 = (A -  $\lambda_0$ )v0
  while  $\|\mathbf{r}_k\| > \tau\|\mathbf{r}_0\|$  do
    Solve Mktk = -rk
    uk+1/2 = uk + tk
    Obtain vk+1 from uk+1/2 and Vk by Gram-Schmidt using  $(\cdot, \cdot)$ 
    Vk+1 = Span(Vk, vk+1)
    Let Pk+1 be the orthogonal projection onto Vk+1
    Find smallest eigenvalue  $\lambda_{k+1}$  and corresponding unit eigenvector w of the restriction of Pk+1APk+1 to Vk+1.
    uk+1 = w
     $k \leftarrow k + 1$ 
    rk = (A -  $\lambda_k$ )uk
  end while
   $\lambda \leftarrow \lambda_k; \mathbf{u} \leftarrow \mathbf{u}_k$ 
```

Our only assumption on the preconditioner in this Hilbert space setting is that M is nonsingular and $M^{-1} : Y \rightarrow X$ continuously. The example in § 3.1 illustrates this setting for an example in which $H = L^2[0, 1]$, $X = C^2[0, 1]$, and $Y = C[0, 1]$.

The three spaces are needed to capture the consistency and stability properties of a finite difference approximation for a differential operator and the Hilbert space nature of the Krylov eigensolver. This, as we explain in § 1.1, is a different, and less straightforward, setting that one needs for nonlinear equations.

In this paper we show that a well-designed (consistent and stable) sequence of approximate problems will track the performance of the infinite dimensional iteration. This is the mesh-independence property [Allgower et al., 1986, Allgower and Böhrer, 1987, Xue, 1995, Kelley and Sachs, 1991, 1992, Ferng and Kelley, 2000] which is well known in the nonlinear solver community.

Mesh-independence theorems are different from convergence theorems. We will illustrate that with the classic result from [Allgower et al., 1986] for nonlinear equations in § 1.1 and again in § 2.1 where we compare a convergence theorem from [Oliveira, 1999] for the generalized Davidson algorithm in the Hermitian case with the mesh-independence in this paper. The convergence results in [Oliveira, 1999] make assumptions that are similar to our stability assumptions.

1.1. Mesh-Independence Results for Nonlinear Equations

Mesh-independence theorems are best known in the setting of nonlinear equations [Willert et al., 2015, Allgower et al., 1986, Allgower and Böhrer, 1987, Ferng and Kelley, 2000, Kelley and Sachs, 1991] and optimization [Kelley and Sachs, 1992, Hintermüller and Ulbrich, 2003]. To illustrate the ideas we will describe one of the results from [Allgower et al., 1986] on Newton’s method. The function space setting is simpler for nonlinear equations case than for the eigenvalue computation in this paper. The reason for this is that we need no scalar product for a Krylov solver in this application. There is only one space X and approximation space X^h .

In the context of nonlinear equations we seek to approximate a nonlinear equation

$$F(u) = 0, \tag{1}$$

on a Banach space X by a sequence of finite dimensional problems

$$\mathbf{F}^h(\mathbf{u}^h) = 0 \tag{2}$$

on finite dimensional spaces X^h with norms $\|\cdot\|_h$. We will refer to h as a mesh parameter. The idea is that the approximation becomes better as $h \rightarrow 0$. We will use a superscript of h for the infinite-dimensional equation when discussing issues that depend on h (Assumption 1.1, for example). We will assume that $\mathbf{F}^h$ is Fréchet differentiable for $h \geq 0$ and denote the Fréchet derivative by $\mathbf{DF}^h$.

Now assume that both the infinite dimensional problem and the sequence of finite dimensional problems satisfy the standard assumptions for quadratic convergence of Newton's method in a mesh-independent manner. Assumption 1.1 makes this precise.

Assumption 1.1. *For all $h \geq 0$ sufficiently small*

1. *There is a solution $\mathbf{u}^{h*}$ of $\mathbf{F}^h(\mathbf{u}^h) = 0$.*
2. *$\mathbf{F}^h$ is Lipschitz continuously Fréchet differentiable with Lipschitz constant γ .*
3. *$\mathbf{DF}^h(\mathbf{u}^{h*})$ is nonsingular and there is M such that*

$$\|(\mathbf{DF}^h)(\mathbf{u}^{h*})^{-1}\|_h \leq M.$$

The classic quadratic convergence estimate [Kelley, 1995] then implies that if the initial error $\|\mathbf{u}^h - \mathbf{u}_0^h\|$ is sufficiently small, then the Newton iteration,

$$\mathbf{u}_{n+1}^h = \mathbf{u}_n^h - (\mathbf{DF}^h)(\mathbf{u}_n^h)^{-1} \mathbf{F}^h(\mathbf{u}_n^h),$$

converges to $\mathbf{u}^{h*}$ and

$$\|\mathbf{u}_{n+1}^h - \mathbf{u}^{h*}\|_h \leq M\gamma \|\mathbf{u}_n^h - \mathbf{u}^{h*}\|_h^2. \quad (3)$$

The uniformity of the estimate (3) in h does not depend on the quality of the approximation, only on the uniform bound for the Lipschitz constant of the derivative and the norm of the inverse of the derivative. This is not a mesh-independent result, but only a (very useful) uniform bound. There is no need for any connection at all between the maps $\mathbf{F}^h$ to obtain (3) other than the uniform bounds on the Lipschitz constant of the derivative and the norm of its inverse.

Mesh independence requires consistency of the approximations $\mathbf{F}^h$ to an underlying “exact” map $\mathbf{F}$. The uniform bounds in Assumption 1.1 can be thought of as stability assumptions. Let $\mathbf{E}^h : X \rightarrow X^h$ be a “discretization” map. The **consistency** assumptions from [Allgower et al., 1986] are

Assumption 1.2. *There are $p \geq 1$ and a neighborhood $\mathcal{N}$ of u^* such that for all $\mathbf{u} \in \mathcal{N}$ and $u, v \in X$,*

1. *$\|\mathbf{F}^h(\mathbf{E}^h u) - \mathbf{E}^h F(u)\| = O(h^p)$ and*
2. *$\|(\mathbf{DF}^h)(\mathbf{E}^h u) \mathbf{E}^h v - \mathbf{E}^h (\mathbf{DF}(u)v)\| = O(h^p)$.*

The theorem from [Allgower et al., 1986] synthesizes two ideas. One is that the consistency assumptions 1.2, the stability assumptions 1.1 for $h = 0$, and the classical Kantorovich theorem [Kantorovich and Akilov, 1982, Kelley, 1995, 2018] imply Assumption 1.1 for h sufficiently small. The other idea, and the core of mesh-independence results, is that the iterations themselves converge. The theorem from [Allgower et al., 1986] is

Theorem 1.1. *Let Assumptions 1.1 (for $h = 0$ only) and 1.2 hold. Then Assumption 1.1 holds for all $h > 0$. The estimate (3) holds, and for $h > 0$ sufficiently small*

$$\mathbf{u}^{h*} - \mathbf{E}^h u^* = O(h^p), \quad (4)$$

$$\mathbf{F}^h(\mathbf{u}_n^h) - \mathbf{E}^h F(u_n) = O(h^p), \text{ and} \quad (5)$$

$$(\mathbf{u}_n^h - \mathbf{u}^{h*}) - \mathbf{E}^h(u_n - u^*) = O(h^p). \quad (6)$$

Our main result Theorem 2.1 is expressed in way similar to the statement of Theorem 1.1.

The mesh-independence result from [Allgower et al., 1986] assumes convergence of the underlying exact iteration, but that is, in fact, not necessary to argue that the conclusions of Theorem 1.1 hold. Moreover, Theorem 1.1 shows that if the exact iteration converges faster than (3) predicts, especially in the early phases of the iteration, then the approximate iteration will reflect that.

The estimates in Theorem 1.1 are only meaningful when the errors in the iteration are larger than the approximation error contained in the O -term. Because of this, many papers that followed [Allgower et al., 1986] express mesh-independence by saying that the index k for which $\mathbf{u}_k^h$ satisfies a termination criterion of the form

$$\|\mathbf{F}^h(\mathbf{u}_k^h)\|/\|\mathbf{F}^h(\mathbf{u}_0^h)\| < \tau \quad (7)$$

is independent of h for h sufficiently small. Corollary 2.1 is our analog of this formulation of mesh-independence. Note that (7) does not depend on convergence order. While the results for nonlinear equations show that p th order accuracy in the equations implies p th order accuracy in the iteration statistics, our results do not. One reason for this is that it is not clear to us how to show that for the preconditioner estimates. Another reason is that many applications, such as the one in § 3.3, do not use a spatial mesh.

In § 2 we state and prove the mesh-independence result. Assumption 2.1 is similar to part 3 of Assumption 1.1 (stability) and Assumption 1.2 (consistency). We do not assume that the operators are Hermitian, as many convergence results do [Ovtchinnikov, 2006, 2003b,a, Oliveira, 1999].

In § 3 we illustrate the results with several examples. The first is a very simple problem that clearly satisfies the assumptions. The second is a non-Hermitian generalized eigenvalue problem from neutron transport theory. The final example is an electronic structure computation where one wants many eigenvalues. We point out that mesh-independence for eigen computations has been observed for certain finite element computations with AMG preconditioning in [Arbenz et al., 2005]. The examples in that paper are consistent with the theory in this paper.

2. Mesh Independence Theorem for the Generalized Davidson Algorithm

We consider a family of discretized finite dimensional linear operators $\{\mathbf{A}^h\}$ and $\{\mathbf{M}^h\}$ on finite dimensional spaces $\{H^h\}$. We put a scalar product $(\cdot, \cdot)_h$ and norm $\|\cdot\|_h$ on H^h . In most of our examples in § 3 the discretization will be nodal, but that is not essential. For example, the example in § 3.3 is a Fourier approximation.

In § 1.1 we made the assumption that the range of F was also the domain of F . We will now consider unbounded operators A and therefore need to extend the evaluation map to Y , the range of A . So we need an evaluation map $\mathbf{E}^h : Y \rightarrow H^h$ in order to specify consistency conditions and a scalar product $(\cdot, \cdot)_h$ on H^h for the orthogonalization in the generalized Davidson iteration.

Our consistency and stability conditions are

Assumption 2.1. *The discretizations are consistent and stable in the sense that*

1. Consistency:

- (a) $\lim_{h \rightarrow 0} \|\mathbf{A}^h \mathbf{E}^h u - \mathbf{E}^h A u\|_h = 0$ for all $u \in X$.
- (b) $\lim_{h \rightarrow 0} (\mathbf{E}^h u, \mathbf{E}^h v)_h = (u, v)_H$ for all $u, v \in Y$.
- (c) $\lim_{h \rightarrow 0} \|\mathbf{A}^h (\mathbf{M}^h)^{-1} \mathbf{E}^h u - \mathbf{A}^h \mathbf{E}^h \mathbf{M}^{-1} u\|_h = 0$ for all $u \in Y$.

2. Stability: There is M_S such that for all h sufficiently small

- (a) $\|(\mathbf{M}^h)^{-1} \mathbf{A}^h\|_h \leq M_S$, $\|\mathbf{A}^h (\mathbf{M}^h)^{-1}\|_h \leq M_S$,
- (b) $\|(\mathbf{A}^h)^{-1}\|_h \leq M_S$, and $\|(\mathbf{M}^h)^{-1}\|_h \leq M_S$.

We will use the following lemma.

Lemma 2.1. *Let Assumption 2.1 hold. Let $u \in X$ with $u \neq 0$. Then*

$$\sigma^h(u) \equiv \mathbf{A}^h \left(\frac{\mathbf{E}^h u}{\|u\|_H} - \frac{\mathbf{E}^h u}{\|\mathbf{E}^h u\|_h} \right) \rightarrow 0 \text{ as } h \rightarrow 0. \quad (8)$$

Proof. Since $u \neq 0$

$$\|\sigma^h(u)\| = \frac{\|\mathbf{A}^h \mathbf{E}^h u\|_h}{\|\mathbf{E}^h u\|_h} \left| \frac{\|\mathbf{E}^h u\|_h}{\|u\|_H} - 1 \right|.$$

and the proof of (8) is complete by part 1b of Assumption 2.1 and the fact that $\|\mathbf{A}^h \mathbf{E}^h u\|_h$ is bounded as $h \rightarrow 0$ because $u \in X$.

□

We will make an assumption on the eigenvalue problem and on the eigensolver in Algorithm 1.

Assumption 2.2. Assume that the eigenvalues λ_k from Algorithm 1 are simple and that the eigensolver used in Algorithm 1 returns a smallest eigenvalue and corresponding unit eigenvector that are continuous functions of the matrix.

Since the eigenvalue is simple, continuity of the eigenvalue follows from standard perturbation theory [Golub and VanLoan, 1996] if the matrix is diagonalizable. The assumption on the unit eigenvector simply says that the eigensolver will not change the sign of the vector for a nearby problem.

Theorem 2.1. Let Assumption 2.1 hold. Suppose the generalized Davidson Algorithm 1 in the infinite dimensional setting with initial iterate u_0 such that $\|u_0\|_H = 1$ has non-zero residuals for the first $K > 0$ iterations.

Let λ_k^h and $\mathbf{r}_k^h$ be the eigenvalues and residuals one obtains from applying Algorithm 1 to the operators $\mathbf{A}^h$ and $\mathbf{M}^h$ with the initial iterate $\mathbf{E}^h u_0$. Then, for all $0 \leq k \leq K$,

$$\lim_{h \rightarrow 0} \|\mathbf{A}^h(\mathbf{u}_k^h - \mathbf{E}^h u_k)\|_h = 0, \quad (9)$$

$$\lim_{h \rightarrow 0} \lambda_k^h \rightarrow \lambda_k, \quad (10)$$

and

$$\lim_{h \rightarrow 0} \|\mathbf{E}^h r_k - \mathbf{r}_k^h\|_h = 0. \quad (11)$$

Proof.

We will verify (10) and (11) inductively. For $k = 0$ the assumption that $\mathbf{u}_0^h = \mathbf{E}^h u_0$ implies that

$$\|\mathbf{A}^h(\mathbf{u}_0^h - \mathbf{E}^h u_0)\|_h = 0, \quad (12)$$

which implies (9) for $k = 0$.

Part 1a of Assumption 2.1 and (12) imply that

$$\begin{aligned} \lambda_0^h &= (\mathbf{A}^h \mathbf{v}_0^h, \mathbf{v}_0^h)_h = \frac{(\mathbf{A}^h \mathbf{E}^h u_0, \mathbf{E}^h u_0)_h}{\|\mathbf{E}^h u_0\|_h^2} \\ &= (\mathbf{A}^h \mathbf{E}^h v_0, \mathbf{E}^h v_0)_h \frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} \\ &= \left((\mathbf{E}^h A v_0, \mathbf{E}^h v_0)_h + ((\mathbf{A}^h \mathbf{E}^h - \mathbf{E}^h A) v_0, \mathbf{E}^h v_0)_h \right) \frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} \end{aligned} \quad (13)$$

Hence

$$\begin{aligned}
\epsilon_0^\lambda(h) &\equiv \lambda_0^h - \lambda_0 = (\mathbf{A}^h \mathbf{v}_0^h, \mathbf{v}_0^h)_h - (Av_0, v_0)_H \\
&= \left((\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h + ((\mathbf{A}^h \mathbf{E}^h - \mathbf{E}^h A)v_0, \mathbf{E}^h v_0)_h \right) \frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} - (Av_0, v_0)_H \\
&= \underbrace{(\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h - (Av_0, v_0)_H}_I + \underbrace{(\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h \left(\frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} - 1 \right)}_{II} \\
&\quad + \underbrace{((\mathbf{A}^h \mathbf{E}^h - \mathbf{E}^h A)v_0, \mathbf{E}^h v_0)_h \frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2}}_{III}.
\end{aligned} \tag{14}$$

We will show that $\lim_{h \rightarrow 0} \epsilon_0^\lambda(h) = 0$ by looking at the three components on the right side of (14).

Beginning with I, since $v_0 \in X \subset Y$, part 1b of Assumption 2.1 implies that

$$\lim_{h \rightarrow 0} (\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h - (Av_0, v_0)_H = 0.$$

Part II is a product of two terms. Firstly

$$\frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} \rightarrow 1$$

as $h \rightarrow 0$ by part 1b of Assumption 2.1. Since

$$\lim_{h \rightarrow 0} (\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h = (Av_0, v_0)_H = \lambda_0$$

by part 1b of Assumption 2.1, we obtain

$$\lim_{h \rightarrow 0} (\mathbf{E}^h Av_0, \mathbf{E}^h v_0)_h \left(\frac{\|u_0\|_H^2}{\|\mathbf{E}^h u_0\|_h^2} - 1 \right) = 0.$$

Finally, we consider III. Since $u_0 \in X$, we have, using part 1a of Assumption 2.1

$$\lim_{h \rightarrow 0} |((\mathbf{A}^h \mathbf{E}^h - \mathbf{E}^h A)u_0, \mathbf{E}^h u_0)_h| \leq \lim_{h \rightarrow 0} \|\mathbf{A}^h \mathbf{E}^h u_0 - \mathbf{E}^h Au_0\|_h \|\mathbf{E}^h u_0\|_h = 0.$$

We will complete the start of the induction by verifying (11) for $k = 0$. Part 1a of Assumption 2.1 and (13) imply that

$$\begin{aligned}
\mathbf{r}_0^h - \mathbf{E}^h r_0 &= \epsilon_0^r(h) \equiv (\mathbf{A}^h \mathbf{u}_0^h - \lambda_0^h \mathbf{u}_0^h) - (\mathbf{E}^h Au_0 - \lambda_0 \mathbf{E}^h u_0) \\
&= \underbrace{(\mathbf{A}^h \mathbf{u}_0^h - \mathbf{A}^h \mathbf{E}^h u_0)}_I + \underbrace{(\mathbf{A}^h \mathbf{E}^h u_0 - \mathbf{E}^h Au_0)}_{II} + \underbrace{\lambda_0 (\mathbf{E}^h u_0 - \mathbf{u}_0^h)}_{III} + \underbrace{(\lambda_0 - \lambda_0^h) \mathbf{u}_0^h}_{IV}.
\end{aligned}$$

To verify (11) for $k = 0$ we must show that $\epsilon_0^r(h) \rightarrow 0$ as $h \rightarrow 0$. We do this by examining each of the four terms separately. The first term (I)

$$\mathbf{A}^h \mathbf{u}_0^h - \mathbf{A}^h \mathbf{E}^h u_0 = 0$$

since $\mathbf{u}_0^h = \mathbf{E}^h u_0$. This also implies that the third term (III)

$$\lambda_0 (\mathbf{E}^h u_0 - \mathbf{u}_0^h)_h = 0.$$

This, in turn, implies that $\|\mathbf{u}_0^h\|$ is bounded as $h \rightarrow 0$, so the fourth term (IV)

$$(\lambda_0 - \lambda_0^h) \mathbf{u}_0^h \rightarrow 0$$

as $h \rightarrow 0$ because we have already verified (10) for $k = 0$. The second term (II)

$$\mathbf{A}^h \mathbf{E}^h u_0 - \mathbf{E}^h A u_0 \rightarrow 0$$

as $h \rightarrow 0$ by Part 1a of Assumption 2.1.

Note Lemma 2.1 implies that

$$\|\mathbf{A}^h \mathbf{v}_0^h - \mathbf{A}^h \mathbf{E}^h \mathbf{v}_0\|_h \rightarrow 0$$

as $h \rightarrow 0$. We will need this to complete the induction.

We can now finish the induction. Assume that for all $l \leq k$

$$\lambda_l^h = \lambda_l + \epsilon_l^\lambda(h), \quad (15)$$

$$\|\mathbf{A}^h \mathbf{u}_l^h - \mathbf{A}^h \mathbf{E}^h u_l\|_h = \epsilon_l^\mathbf{u}(h), \quad (16)$$

and

$$\|\mathbf{A}^h \mathbf{v}_l^h - \mathbf{A}^h \mathbf{E}^h v_l\|_h = \epsilon_l^\mathbf{v}(h), \quad (17)$$

where

$$\lim_{h \rightarrow 0} \epsilon_l^\lambda(h) = \lim_{h \rightarrow 0} \epsilon_l^\mathbf{u}(h) = \lim_{h \rightarrow 0} \epsilon_l^\mathbf{v}(h) = 0. \quad (18)$$

Similarly to the $k = 0$ case, (15), (16), and (18) imply that for all $0 \leq l \leq k$

$$\epsilon_l^\mathbf{r}(h) \equiv \|\mathbf{r}_l^h - \mathbf{E}^h r_l\|_h \rightarrow 0 \quad (19)$$

as $h \rightarrow 0$. We will verify that (15) and (17) hold for iteration $k + 1$ and thereby complete the proof.

After computing $\mathbf{r}_k^h$ we apply the preconditioner to obtain

$$\begin{aligned} \mathbf{t}_k^h &= -(\mathbf{M}^h)^{-1} \mathbf{r}_k^h = -(\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k) - (\mathbf{M}^h)^{-1} \mathbf{E}^h r_k \\ &= -(\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k) - ((\mathbf{M}^h)^{-1} \mathbf{E}^h r_k - \mathbf{E}^h M^{-1} r_k) - \mathbf{E}^h M^{-1} r_k \\ &= \mathbf{E}^h t_k - (\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k) - ((\mathbf{M}^h)^{-1} \mathbf{E}^h r_k - \mathbf{E}^h M^{-1} r_k). \end{aligned} \quad (20)$$

Let

$$\epsilon_k^\mathbf{t}(h) = \|\mathbf{A}^h (\mathbf{t}_k^h - \mathbf{E}^h t_k)\|_h.$$

We use (20) to obtain

$$\begin{aligned} \epsilon_k^\mathbf{t}(h) &= \|\mathbf{A}^h (\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k) - \mathbf{A}^h ((\mathbf{M}^h)^{-1} \mathbf{E}^h r_k - \mathbf{E}^h M^{-1} r_k)\|_h \\ &\leq \|\mathbf{A}^h (\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k)\|_h + \|\mathbf{A}^h ((\mathbf{M}^h)^{-1} \mathbf{E}^h r_k - \mathbf{E}^h M^{-1} r_k)\|_h. \end{aligned} \quad (21)$$

We will analyze the two components on the right side of (21) separately. Note that part 2 of Assumption 2.1 and (19) imply that

$$\lim_{h \rightarrow 0} \|\mathbf{A}^h (\mathbf{M}^h)^{-1} (\mathbf{r}_k^h - \mathbf{E}^h r_k)\|_h = 0.$$

Moreover, since $r_k \in Y$, Part 1c implies that

$$\lim_{h \rightarrow 0} \|\mathbf{A}^h ((\mathbf{M}^h)^{-1} \mathbf{E}^h r_k - \mathbf{E}^h M^{-1} r_k)\|_h = 0.$$

Therefore $\epsilon_k^\mathbf{t}(h) \rightarrow 0$ as $h \rightarrow 0$.

The next step is orthogonalizing $\mathbf{u}_{k+1/2} = \mathbf{u}_k + \mathbf{t}_k$ against the previous basis vectors. Using (21) and (16) we obtain

$$\lim_{h \rightarrow 0} \|\mathbf{A}^h \mathbf{u}_{k+1/2}^h - \mathbf{A}^h \mathbf{E}^h u_{k+1/2}\|_h = 0. \quad (22)$$

Now $v_{k+1} = w_{k+1}/\|w_{k+1}\|_H$ where

$$w_{k+1} = u_{k+1/2} - \sum_{l=0}^k (u_{k+1/2}, v_l)_H v_l. \quad (23)$$

Similarly $\mathbf{v}_{k+1}^h = \mathbf{w}_{k+1}/\|\mathbf{w}_{k+1}\|_h$ where

$$\mathbf{w}_{k+1}^h = \mathbf{u}_{k+1/2}^h - \sum_{l=0}^k (\mathbf{u}_{k+1/2}^h, \mathbf{v}_l^h)_h \mathbf{v}_l^h, \quad (24)$$

and $\mathbf{v}_{k+1}^h = \mathbf{w}_{k+1}^h/\|\mathbf{w}_{k+1}^h\|_h$. Our next task is to show that

$$\|\mathbf{A}^h(\mathbf{v}_{k+1}^h - \mathbf{E}^h v_{k+1})\|_h \rightarrow 0 \text{ as } h \rightarrow 0. \quad (25)$$

This will follow from

$$\|\mathbf{A}^h(\mathbf{w}_{k+1}^h - \mathbf{E}^h w_{k+1})\|_h \rightarrow 0 \text{ as } h \rightarrow 0, \quad (26)$$

because (26) and (8) will imply (25).

We begin by noting that

$$\lim_{h \rightarrow 0} (\mathbf{u}_{k+1/2}^h, \mathbf{v}_l^h)_h = (u_{k+1/2}, v_l)_H \quad (27)$$

for all $0 \leq l \leq k$ by the induction hypotheses, (16) (21). Then we may use (23), (24), and (17) to obtain (26).

The eigenvalue λ_{k+1} is the smallest eigenvalue of the matrix $\mathcal{A}$ with entries

$$(\mathcal{A})_{ij} = (Av_i, v_j)_H.$$

Similarly λ_{k+1}^h is the smallest eigenvalue of the matrix $\mathcal{A}^h$ with entries

$$(\mathcal{A}^h)_{ij} = (\mathbf{A}^h \mathbf{v}_i^h, \mathbf{v}_j^h)_h.$$

Convergence of the $\mathbf{v}$ s in the sense of (17) and (25) and parts 1a and 1b of Assumption 2.1 imply that

$$\lim_{h \rightarrow 0} \mathcal{A}_{ij}^h = \mathcal{A}_{ij}.$$

Assumption 2.2 then implies that the eigenvalue converges

$$\lim_{h \rightarrow 0} \lambda_{k+1}^h = \lambda,$$

verifying (15) for $l = k + 1$. Moreover the eigenvector $\mathbf{z}_{k+1}^h$ corresponding to λ_{k+1}^h also converges

$$\lim_{h \rightarrow 0} \mathbf{z}_{k+1}^h = \mathbf{z}_{k+1}.$$

This completes the proof since we can expand $\mathbf{u}_{k+1}^h$ and u_{k+1} as

$$\mathbf{u}_{k+1}^h = \sum_{j=1}^{k+1} z_j^h \mathbf{v}_j^h \text{ and } u_{k+1} = \sum_{j=1}^{k+1} z_j v_j,$$

where $\mathbf{z}_{k+1} = (z_1, \dots, z_{k+1})^T$ and $\mathbf{z}_{k+1}^h = (z_1^h, \dots, z_{k+1}^h)^T$. Therefore

$$\begin{aligned} \mathbf{A}^h(\mathbf{u}_{k+1}^h - \mathbf{E}^h u_{k+1}) &= \sum_{j=1}^{k+1} z_j \mathbf{A}^h(\mathbf{v}_j^h - \mathbf{E}^h v_j) \\ &\quad + \sum_{j=1}^{k+1} (z_j^h - z_j) \mathbf{A}^h \mathbf{E}^h v_j \rightarrow 0 \end{aligned} \quad (28)$$

as $h \rightarrow 0$ by the convergence of the eigenvectors and (17). $\square$

The mesh-independence result Theorem 2.1 requires the stability and consistency assumptions 2.1 and assumes that the infinite dimensional iteration converges. We now prove Corollary 2.1, which states that if the infinite dimensional iteration does terminate successfully with a small residual, then the approximate iteration will do so as well in the same number of iterations.

Corollary 2.1. *Let the assumptions of Theorem 2.1 hold. If the infinite dimensional Davidson iteration terminates for a given $\tau > 0$ after exactly K iterations with $r_K \neq 0$, Then for all h sufficiently small, the generalized Davidson algorithm applied to $\mathbf{A}^h$ with initial vector $\mathbf{E}^h u_0$ will also terminate after K iterations.*

Proof. Suppose K is the first index for which $\|r_k\|_H < \tau \|r_0\|_H$.

We can use (11) from Theorem 2.1 implies that (11) holds to complete the proof since for all $0 \leq k \leq K$

$$|\|\mathbf{r}_k^h\|_h - \|r_k\|_H| \leq |\|\mathbf{r}_k^h\|_h - \|\mathbf{E}^h r_k\|_h| + |\|\mathbf{E}^h r_k\|_h - \|r_k\|_H| \leq \epsilon_k^r(h) + \|\mathbf{E}^h r_k\|_h - \|r_k\|_H \rightarrow 0 \quad (29)$$

as $h \rightarrow 0$ by (11) and Part 1b of Assumption 2.1. Hence (29) implies that K is also the first K for which $\|\mathbf{r}_k^h\|_h < \tau \|\mathbf{r}_0^h\|_h$.

$\square$

The stability assumption on the discretization (Part 2b of Assumption 2.1) is not used directly in the proof of Theorem 2.1, but an unstable discretization, even if consistent, will not converge and the theorem would be meaningless in that event. We also note that if one only considers a finite number K of iterations, then one can weaken the assumption on convergence of the infinite dimensional iteration (Assumption 2.2) to only assume that the infinite dimensional iteration does not terminate prematurely with a zero residual. In this way our results apply even to divergent iterations.

2.1. Convergence Results are Different from Mesh Independence

In the analysis for mesh-independence we do not assume any symmetry for $\mathbf{A}$ or $\mathbf{M}$ or even that the iteration converges. However, some convergence results make assumptions similar to ours and we will discuss one such result in this section. In [Oliveira, 1999] the objective is to find the smallest eigenvalue λ^* and corresponding eigenvector $\mathbf{u}^*$ for a symmetric positive definite matrix $\mathbf{A}$ with the generalized Davidson algorithm using the symmetric positive definite preconditioner $\mathbf{M}$. The convergence result requires a stability assumption.

Assumption 2.3. *$\mathbf{M}$ and $\mathbf{A}$ are symmetric positive definite. $\mathbf{M}$ is held fixed for the entire iteration (i. e. independent of the current approximation to the eigenvalue). The smallest eigenvalue λ^* of $\mathbf{A}$ is strictly less than the second smallest λ_2 . There is $c > 0$ such that*

$$\|\mathbf{M}^{-1}\mathbf{A}\| \leq c \text{ and } \|(\mathbf{M}^{-1}\mathbf{A})^{-1}\| \leq c. \quad (30)$$

Note that (30) implies that $\kappa((\mathbf{M})^{-1}\mathbf{A}) \leq c^2$.

The result from [Oliveira, 1999] is

Theorem 2.2. *Let Assumption 2.3 hold. Then the generalized Davidson iteration $(\{\lambda_k\}, \{\mathbf{u}_k\})$ converges to $(\lambda^*, \mathbf{u}^*)$ in the sense that*

$$\limsup_{k \rightarrow \infty} \frac{|\lambda_{k+1} - \lambda^*|}{|\lambda_k - \lambda^*|} \leq \sigma^2 \quad (31)$$

and

$$\limsup_{k \rightarrow \infty} \frac{\angle(\mathbf{u}_{k+1}, \mathbf{u}^*)}{\angle(\mathbf{u}_k, \mathbf{u}^*)} \leq \sigma. \quad (32)$$

Here $\angle(\mathbf{u}, \mathbf{v})$ is the angle between the subspaces spanned by the vectors $\mathbf{u}$ and $\mathbf{v}$ and

$$\sigma = \frac{1 - (1 - \rho)/c^2}{1 + (1 - \rho)/c^2}.$$

Part 2 of Assumption 2.1 is similar, but weaker, than Assumption 2.3. The convergence results in [Oliveira, 1999] only depend on stability of the preconditioner and the ratio of the smallest eigenvalue λ^* and the next smallest λ_2

$$\rho = \lambda^*/\lambda_2.$$

Our assumptions could be expanded to require that the bounds needed for Theorem 4.1 in [Oliveira, 1999] hold for all h . If we did that then, in the symmetric positive definite case, the convergence bounds for that theorem would be independent of h . However, these are worst-case bounds and are asymptotic results, similar to those for Newton's methods, where the standard assumptions imply (3), which is an asymptotic bound. Contrast this to mesh-independence, where the result is that the performance of the first given number of iterations converges as $h \rightarrow 0$.

Suppose the assumptions for Theorem 2.2 hold for the families of approximations $\{\mathbf{A}^h\}$ and $\{\mathbf{M}^h\}$ independently of h . Then the convergence of the generalized Davidson iterations will all have the asymptotic behavior given by (31) and (32). This does not imply mesh-independence, which is a property of the entire iteration. It is interesting to note that [Oliveira, 1999] presents results (Figure 1) that show mesh-independence, even though the theory only predicts asymptotic convergence rates. This paper explains those observations in more detail.

The example in § 3.1 satisfies Assumption 2.3 in a mesh-independent way.

2.2. Generalized Eigenvalue Problem

The results in § 2 extend directly to the generalized eigenvalue problem

$$\mathbf{A}\mathbf{u} = \lambda\mathbf{B}\mathbf{u}, \tag{33}$$

where $\mathbf{B}$ is nonsingular. The convergence results in [Ovtchinnikov, 2003b,a] include Hermitian positive definite instance of this case.

The unfortunately named generalized Davidson algorithm for the generalized eigenvalue problem [Morgan, 1990] is

Algorithm 2 Generalized Davidson Algorithm for GEP

$(\mathbf{v}, \lambda) = \text{davidson_gep}(\mathbf{u}_0, \mathbf{A}, \mathbf{B}, \mathbf{M}, \tau)$

$k = 0$

$\mathbf{v}_0 = \mathbf{u}_0 / \|\mathbf{u}_0\|_H$

$\mathbf{V}_0 = \text{Span}(\mathbf{v}_0)$

$\lambda_0 = (\mathbf{v}_0, \mathbf{A}\mathbf{v}_0)_H / (\mathbf{v}_0, \mathbf{B}\mathbf{v}_0)_H$

$\mathbf{r}_0 = (\mathbf{A} - \lambda_0\mathbf{B})\mathbf{v}_0$

while $\|\mathbf{r}_k\|_H > \tau\|\mathbf{r}_0\|_H$ **do**

 Solve $\mathbf{M}_k\mathbf{t}_k = -\mathbf{r}_k$

$\mathbf{u}_{k+1/2} = \mathbf{u}_k + \mathbf{t}_k$

 Obtain $\mathbf{v}_{k+1}$ from $\mathbf{u}_{k+1/2}$ and $\mathbf{V}_k$ by Gram-Schmidt using $(\cdot, \cdot)_H$

$\mathbf{V}_{k+1} = \text{Span}(\mathbf{V}_k, \mathbf{v}_{k+1})$

 Let P_{k+1} be the orthogonal projection onto $\mathbf{V}_{k+1}$

 Find smallest eigenvalue λ_{k+1} and corresponding unit eigenvector $\mathbf{w}$ for the problem $P_{k+1}\mathbf{A}P_{k+1}\mathbf{w} = \lambda_{k+1}P_{k+1}\mathbf{B}P_{k+1}\mathbf{w}$.

$\mathbf{u}_{k+1} = \mathbf{w}$

$k \leftarrow k + 1$

$\mathbf{r}_k = (\mathbf{A} - \lambda_k\mathbf{B})\mathbf{u}_k$

end while

Theorem 2.1 holds for this algorithm if we include $\mathbf{B}$ in the consistency and stability assumptions. We would assume that

$$\|\mathbf{B}^h E^h u - E^h \mathbf{B} u\|_h \rightarrow 0 \text{ as } h \rightarrow 0 \text{ for all } u \in X. \tag{34}$$

and

$$\|(\mathbf{M}^h)^{-1} \mathbf{B}^h\|_h \text{ is uniformly bounded in } h. \tag{35}$$

3. Examples

We present four examples to illustrate the theory. We begin in § 3.1 with a simple eigenvalue problem where Assumption 2.1 is trivially satisfied. The second in § 3.2 is a generalized eigenvalue problem from computational neutronics. The operator in § 3.2 is non-symmetric. The final examples are from electronic structure computations with two different approximations: a plane wave basis in § 3.3 and a real space discretization in § 3.4.

3.1. Integro-differential Equation in One Dimension

We will find the smallest eigenvalue of A , where

$$Au(x) = -u''(x) + \int_0^1 k(x, y)u(y) dy.$$

and

$$k(x, y) = -e^{|x-y|/2}.$$

The domain of A is

$$X = \{u \mid u \in C^2[0, 1], u(0) = u(1) = 0\}.$$

The range is $Y = C[0, 1]$ and the Hilbert space scalar product for orthogonalization is $L^2[0, 1]$ with the usual L^2 scalar product. Our preconditioner is the inverse of the second derivative term in the operator.

$$Mu(x) = -u''(x).$$

Clearly $M^{-1} : Y \rightarrow X$ as is needed for the terms in the generalized Davidson algorithm to be defined.

We discretized the differential operator with the standard central difference scheme and used the trapezoid rule for the integral operator. We use an equally spaced grid with N interior grid points and $h = 1/(N + 1)$. The evaluation map E^h is evaluation at the nodes of the difference scheme. With these choices the consistency hypotheses hold with the norm on X being the L^∞ norm.

Note that A^h and M^h are Hermitian and that M does not depend on the current approximation to λ . It is easy to verify that Assumption 2.3 holds with c and λ^*/λ_2 independent of h for h sufficiently small. Similarly, Assumption 2.1 follows from well-known properties of the central difference discretization [LeVeque, 2007] and the trapezoid rule discretization of integral operators [Anselone, 1971].

The initial iterate was $v = u_0/\|u_0\|_H$ where $u_0(x) = x(1 - x)$. v was discretized by evaluation at the mesh points.

In Table 1 we report on the relative residual histories for the generalized Davidson iteration for five different values of the mesh spacing h . We terminated the iteration when the residual was smaller than 10^{-6} . The mesh-independence of the iteration is clearly evident, even in the third figure of the residuals. We tabulate the residual histories in the discrete L^2 norm

$$\|\mathbf{r}\| = \left(h \sum_{i=1}^N r_i^2 \right)^{1/2}.$$

Table 1: Relative Residual Histories

h=1/1000	h=1/2000	h=1/4000	h=1/8000	h=1/16000
1.0000e+00	1.0000e+00	1.0000e+00	1.0000e+00	1.0000e+00
6.0495e-02	6.0632e-02	6.0700e-02	6.0734e-02	6.0751e-02
1.3359e-03	1.3433e-03	1.3470e-03	1.3488e-03	1.3498e-03
1.5032e-05	1.5179e-05	1.5253e-05	1.5290e-05	1.5310e-05
1.0224e-07	1.0380e-07	1.0460e-07	1.0533e-07	1.0736e-07

3.2. Neutron transport: Generalized Eigenvalue Problem

In this section, we consider the solution of the k -eigenvalue form of the neutron transport equation. This equation can be written as

$$\hat{\Omega} \cdot \nabla \psi + \sigma \psi = \int_0^\infty dE \int_{4\pi} d\hat{\Omega} \sigma_s \psi + \frac{1}{k} \chi \int_0^\infty dE \int_{4\pi} d\hat{\Omega} \nu \sigma_f \psi, \quad (36)$$

where $\hat{\Omega}$ is the neutron direction, E is the neutron energy, $\psi(\vec{r}, \hat{\Omega}, E)$ is the angular flux, $\sigma(\vec{r}, E)$ is the total cross section, $\sigma_s(\vec{r}, \hat{\Omega}' \rightarrow \hat{\Omega}, E' \rightarrow E)$ is the scattering cross section, $\chi(\vec{r}, E)$ is the fission energy distribution, $\nu(\vec{r}, E)$ is the number of neutrons produced per fission event, and $\sigma_f(\vec{r}, E)$ is the fission cross section. The eigenvalue k represents the multiplication factor of the system— k less than one corresponds to a neutron population that is decreasing in time, k greater than one corresponds to a population increasing in time, and k exactly equal to one corresponds to a constant population. The quantity that is sought is the largest magnitude eigenvalue k (commonly known in the literature as k -effective) and the corresponding eigenvector. It is known that the dominant eigenvalue is real, positive, and simple and the corresponding eigenvector is everywhere nonnegative [Borysiewicz and Mika, 1972]. This problem can be written in operator notation as

$$(\mathbf{T} - \mathbf{S})\psi = \frac{1}{k} \mathbf{F}\psi, \quad (37)$$

where $\mathbf{T}$ is the streaming-plus-collision operator, $\mathbf{S}$ is the scattering operator, and $\mathbf{F}$ is the fission operator. The operator $\mathbf{T}$ is guaranteed to be nonsingular [Faber and Manteuffel, 1988], which permits rewriting (37) in integral form as

$$(\mathbf{I} - \mathbf{T}^{-1}\mathbf{S})\psi = \frac{1}{k} \mathbf{T}^{-1}\mathbf{F}\psi. \quad (38)$$

The transport equation must be discretized in energy, angle, and space. The multigroup approximation is the energy discretization employed by every major production radiation transport solver [Lewis and Miller, 1993], and will be used in this study. Radiation transport solvers are primarily classified by the type of angular discretization used. In the spherical harmonics, or P_N , method, the angular dependence of the solution is expanded in spherical harmonic moments. The diffusion approximation to the transport equation can be derived from a two-term truncation of the spherical harmonics expansion. The other main angular discretization is the discrete ordinates, or S_N , method [Carlson and Lathrop, 1965]. The discrete ordinates method is an angular collocation method where the transport equation is enforced for a finite number of directions. Integrals in angle are approximated using quadrature rules. Quadrature sets defining the discrete angles and corresponding quadrature weights are usually selected to satisfy certain symmetry and accuracy criteria (such as integrating the maximum possible number of spherical harmonic functions for a given number of angles). For discretization of the spatial variable, finite difference, finite element, and finite volume methods are all in widespread use [Hamilton, 2011].

In this work we consider the method of characteristics (MOC) formulation of the radiation transport equation [Askew, 1972], which falls into the discrete ordinates family of methods. The MOC approach divides a problem geometry into a set of spatial cells in which the scattering and fission sources are assumed to be constant (although linear source versions of MOC do exist [Ferrer et al., 2012]). For each angle, a set of rays are traced from one domain boundary to the opposite boundary; the transport equation is solved analytically within each constant-source region. Because of its ability to naturally handle curvilinear and complex geometries, the MOC equations are commonly used for analysis of nuclear reactors, which commonly consist of numerous cylindrical fuel elements. The MOC formulation is almost exclusively used for two-dimensional problems, as the computational requirements for the three-dimensional extension render it uncompetitive with other methods.

In the case of energy-independent transport, the integral operator $(\mathbf{I} - \mathbf{T}^{-1}\mathbf{S})$ has been shown to be self-adjoint, positive, and a compact perturbation of the identity (cf. [Faber and Manteuffel, 1988] in a single spatial dimension and [Scheben and Graham, 2011] in multiple dimensions). Methods based on the discrete ordinates angular discretization generally do not maintain the self-adjoint property of the continuous problem, although Chang introduced an approach that allows the property to be retained with certain restrictions on the quadrature set [Chang, 2007]. This study also observed mesh-independent convergence for linear systems involving the energy-independent transport equation using the conjugate gradient method. The spectral radius of the operator $\mathbf{T}^{-1}\mathbf{S}$ is less than unity, as demonstrated in [Faber and Manteuffel, 1988] for the continuous problem, [Greenbaum, 1997] for a finite-difference discretized system, and [Chang, 2007] for a finite-element discretization. [The energy-dependent case is not self-adjoint due to the structure of](#)

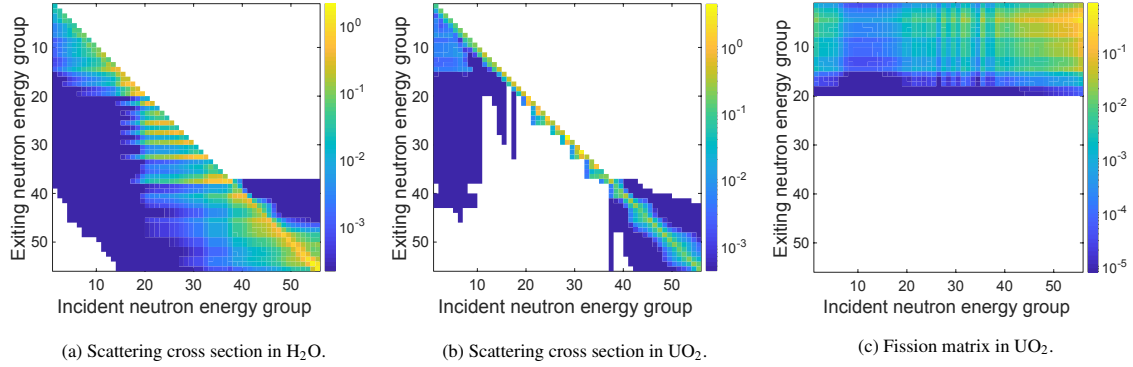


Figure 1: 56-group cross section data for two common materials. Scattering cross section corresponds to $\mathbf{S}$ and the fission matrix corresponds to $\mathbf{F}$ in (38). Energy group 1 represents the highest energy and group 56 is the lowest energy.

the matrices $\mathbf{S}$ and $\mathbf{F}$. Examples of the cross section data for two materials are provided in Fig. 1. This data determines the block structure of the matrices $\mathbf{S}$ and $\mathbf{F}$ in (38). It is evident that the data introduces a significant amount of asymmetry into the system, with most entries in the scattering matrices being located on or below the main diagonal and all entries in the fission matrix beyond group 20 are zero. Also note that the fission matrix is identically zero for any spatial cell not containing a fuel material. As noted in § 2, our convergence results do not rely on the operators being Hermitian.

For this work, we use the radiation transport solver within the POLARIS code [Jessee et al., 2014], a reactor analysis package developed at Oak Ridge National Laboratory. As a test problem, we choose a model of an assembly from the Takahama pressurized water reactor as described in [Radulescu et al., 2010]. Due to the presence of strongly absorbing materials, this was noted to be a challenging problem to converge. Five different problem resolutions are proposed in which the space and angular variables are simultaneously refined. These parameters, as well as the corresponding computed k -effective values, are provided in Table 2. A 56-group cross section library is used in all cases; this library is a standard choice for reactor analyses. The discretized problem geometries for two different spatial resolutions are shown in Fig. 2. A generalized Davidson eigensolver from the Trilinos library [Heroux et al., 2003] is used, solving (38) using Algorithm 2. The preconditioner is taken to be a fixed number of Richardson iterations, corresponding to the preconditioner

$$\mathbf{M}^{-1} = \sum_{n=0}^N (\mathbf{T}^{-1}\mathbf{S})^n. \quad (39)$$

The initial guess in all cases is a constant vector.

The correspondence with the general description in § 2.2 is $\lambda = 1/k$,

$$\mathbf{A} = \mathbf{I} - \mathbf{T}^{-1}\mathbf{S}, \text{ and } \mathbf{B} = \mathbf{T}^{-1}\mathbf{F}.$$

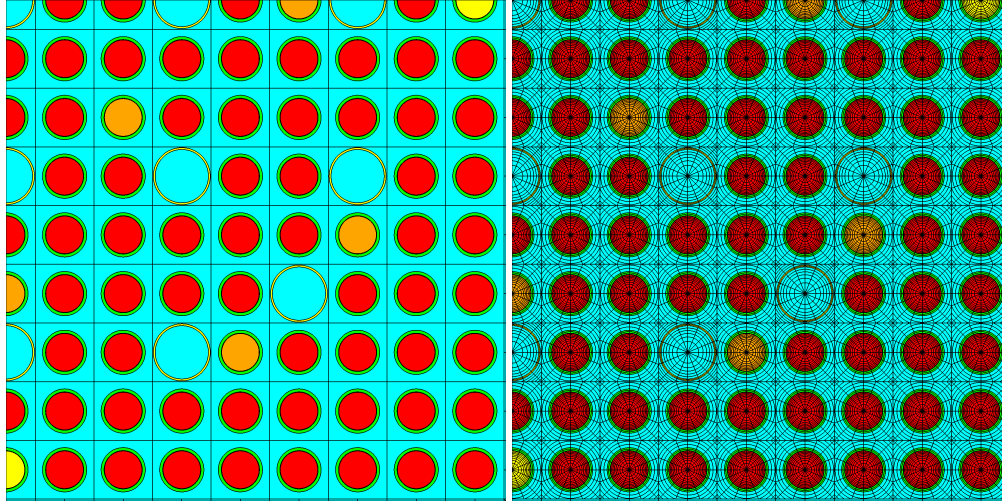
Consistency properties equivalent to parts 1a and 1b of Assumption 2.1 for the discretized radiation transport equation are well documented for common discretizations [Lesaint and Raviart, 1974, Pitkäranta and Scott, 1983, Johnson and Pitkäranta, 1983]. These results also imply (34), as the only mesh dependence in $\mathbf{B}$ is contained in $\mathbf{T}$, which appears identically in $\mathbf{A}$ and $\mathbf{B}$. As noted previously, $\rho(\mathbf{I} - \mathbf{A}) \equiv \rho(\mathbf{T}^{-1}\mathbf{S}) < 1$. Because $\mathbf{M}^{-1}$ only involves powers of the operator $(\mathbf{I} - \mathbf{A})$, parts 1c, 2, and the final statement in 2b of Assumption 2.1 will be satisfied, as will (35). For the purposes of this study, the energy discretization will be fixed and is therefore not a factor in the consistency and stability considerations.

Table 3 shows the number of iterations required for convergence using either one or five iterations of Richardson iteration. The use of additional Richardson iterations in the preconditioner results in a smaller number of Davidson iterations. For both preconditioners, the iteration count is essentially independent of the level of resolution.

Figure 3 shows the convergence behavior for the Davidson eigenvalue solver for three different mesh resolutions. The preconditioner for this case is five Richardson iterations. Some slight variation in behavior is observed, particularly

Table 2: Discretization parameters for Takahama PWR assembly problem.

Discretization level	Cells	Angles	Ray spacing (cm)	Total segments	k -effective
1	807	4	0.08	13,167	1.118783
2	2009	16	0.04	80,572	1.113687
3	5716	32	0.02	552,494	1.116683
4	17,076	96	0.01	3,546,452	1.119555
5	58,598	192	0.005	24,524,659	1.121148



(a) Level 1 mesh.

(b) Level 4 mesh.

Figure 2: Representative spatial meshes for Takahama PWR assembly.

in the first few iterations, but the average rate of convergence is nearly identical across all resolutions. This behavior is consistent with the expectation that the convergence of the Davidson method is asymptotically independent of the discretization level.

Table 3: Davidson eigenvalue iterations to convergence for Takahama PWR assembly.

Discretization level	Preconditioner	
	1 Richardson	5 Richardsons
1	32	13
2	31	12
3	31	12
4	31	12
5	31	13

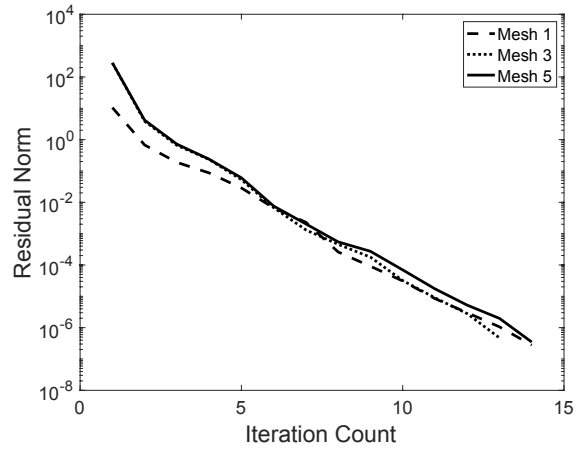


Figure 3: Davidson convergence history for solution of k -eigenvalue problem for three different mesh resolutions.

3.3. Electronic Structure Computation: Plane Wave Discretization

We consider solving the Kohn-Sham (KS) eigenvalue problem of the form

$$H(\rho)\psi_i(\mathbf{r}) = \psi_i(\mathbf{r})\varepsilon_i, \quad (40)$$

where $\varepsilon_1 \leq \varepsilon_2 \leq \dots \varepsilon_{n_e}$ are the n_e algebraically smallest eigenvalues of the Kohn-Sham Hamiltonian $H(\rho)$ which is a function of the electron density ρ defined in term of desired eigenfunctions of H .

$$\rho(\mathbf{r}) = \sum_{i=1}^{n_e} |\psi_i(\mathbf{r})|^2.$$

Because H depends on the eigenfunctions to be computed, this is a nonlinear eigenvalue problem that must be solved by a nonlinear iterative method. The most widely used method is the self-consistent field (SCF) iteration in which a sequence of linear eigenvalue problems for fixed electron densities ρ are solved. The computed eigenfunction approximations are used to update ρ for the subsequent SCF iteration.

In this section, we solve the Kohn-Sham equation for the Buckminsterfullerene (i.e., the C60 molecule, see Figure 4). We discretize the KS equation (40) by expanding ψ_i in planewaves $e^{i\mathbf{G}\cdot\mathbf{r}}$, where $\mathbf{G}$ is a vector in the reciprocal space of a unit (super)cell Ω that contains the C60 molecule. We choose the supercell to be $[0, 20] \times [0, 20] \times [0, 20]$ (in Bohr).

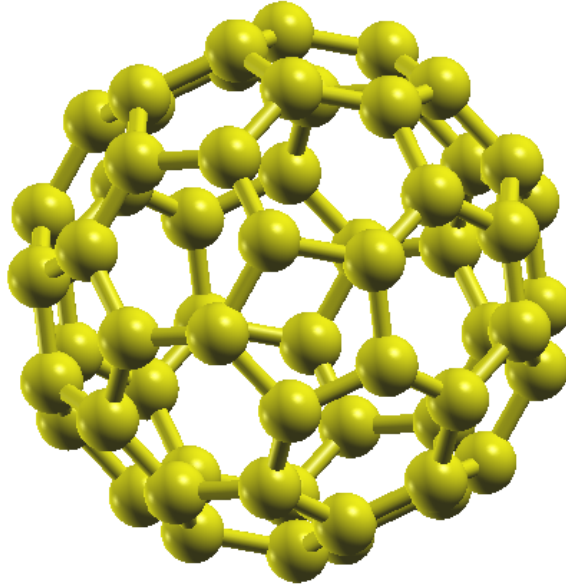


Figure 4: The C60 molecule.

The accuracy of the discretization is determined by the planewave cutoff parameter E_{cut} . i.e., we only include planewaves that satisfy

$$\|\mathbf{G}\|^2/2 < E_{cut}.$$

The larger the E_{cut} , the more accurate the discretization and the larger the dimension of the discretized problem.

Because the KS Hamiltonian has the form

$$H = -\frac{1}{2}L + V(\rho(\mathbf{r})), \quad (41)$$

where L is the Laplacian operator and V is a potential operator that consists of an low rank non-local ionic pseudo-potential term as well as local ionic pseudo-potential, Hartree and exchange-correlation terms, multiplying H with

a vector can be performed efficiently by representing L and the non-local part of the ionic pseudo-potential in the reciprocal space and the rest of V in the real space, and using the fast Fourier transform (FFT) to move the vector back and forth between these two spaces. We do not explicitly construct H as a matrix because it is dense in both the real and reciprocal space.

It is well known that a suitable preconditioner T for the generalized Davidson algorithm is the inverse of a modified Laplacian [Teter et al., 1989] that can be efficiently applied in the reciprocal space.

The *a priori* error analysis of the planewave approximation of the Kohn-Sham model using pseudopotentials has been analyzed in [Cancès et al., 2012]. For a fixed system size with increasingly refined mesh, we expect that the Assumptions 2.1 are satisfied with the preconditioner used here [Teter et al., 1989], as indicated from the mesh-independent results below.

In the planewave discretization, E^h projects a function to the span of Fourier modes within a kinetic energy cutoff. Since the Fourier basis set is a complete basis set, Assumption 2.1 Consistency (a), (b) hold naturally. The Teter preconditioner M commutes with E^h , and furthermore $E^h M^{-1} = (M^h)^{-1} E^h$, which gives 2.1 consistency (c). Regarding the stability, the Teter preconditioner is again chosen so that the divergence of the Laplacian operator as $h \rightarrow 0$ is precisely canceled, so that Stability (a) is satisfied by design. It is also by design that the Teter preconditioner satisfies $\|(M^h)^{-1}\| \leq M_S$. Finally $\|(A^h)^{-1}\| \leq M_S$ can always be satisfied by shifting the matrix A^h . This gives the Stability (b).

We use the KSSOLV software package [Yang et al., 2009] to perform a spin-unpolarized calculation for the C60 molecule using the Optimized Norm-Conserving Vanderbilt (ONCV) pseudopotential [Hamann, 2013] to model the ionic core potential and the Perdew-Zunger local density exchange-correlation functional [Perdew and Zunger, 1981]. Because each C atom has 4 valence electrons (two valence electron pairs), the total number of eigenvalues to be computed is 120.

We use three different planewave energy cutoffs to discretize the Kohn-Sham equation: $E_{cut} = 6.25, 12.25, 25$ Hartree. For each discretized problem, we compute the 2-norm of the preconditioned Hamiltonian $T^{-1}H$. We observe that in each case, $\|T^{-1}H\|_2$ is around 0.92.

We demonstrate the convergence of the Davidson and LOBPCG algorithms [Knyazev, 2001] using the initial KS Hamiltonian constructed at the beginning of the SCF cycle. The initial approximation (iterate) is chosen to be a set of i.i.d, random numbers drawn from $N(0,1)$ distribution, orthonormalized by a QR factorization.

Our implementation of the Davidson algorithm only keeps the current approximation to the desired eigenvectors and the preconditioned residuals in the search space to reduce memory usage. The Davidson iteration is restarted with the most recent approximation to the desired eigenvectors in each step. LOBPCG is the default eigensolver in KSSOLV. It is equivalent to restarted Davidson that keeps two sets of previous approximations (setting maximum of k to 3 in Algorithm 1 and restart when convergence is not reached). These examples show that restart has no effect on mesh independence of convergence. The theory predicts this since the restarted iteration can be viewed as a separate iteration with a new initial iterate and Theorem 2.1 can be applied to that new iteration. The electron density ρ used to construct such a Hamiltonian is obtained by taking the superposition of atomic electron densities of all 60 carbon atoms and normalizing the density to have the correct electron charge. A random starting guess is used in each Davidson/LOBPCG run.

In Figure 5, we plot the change of eigenspace residual norm defined as

$$\|R\|_F = \|HX - X\Lambda\|_F,$$

where $\|\cdot\|_F$ is the Frobenius norm, X contains the reciprocal space representation of the approximated eigenvectors $\{\psi_i(\mathbf{r})\}$, i.e. their planewave expansion coefficients, and Λ is a diagonal matrix containing the corresponding eigenvalues, with respect to the number of Davidson iterations.

We clearly see from this figure that the convergence rate of the generalized Davidson algorithm is nearly independent of the planewave cutoff value E_{cut} . The nearly E_{cut} -independent convergence rate can also be observed in Figure 6 for the LOBPCG algorithm. The LOBPCG algorithm converges faster because its search space contains contributions from two most recent approximations to the desired eigenspace.

3.4. Electronic Structure Computation: Real Space Discretization

The Kohn-Sham (KS) equation (40) described in the previous section may be discretized using an alternate representation that uses regular real space grids in place of plane waves [Briggs et al., 1996]. This formulation allows

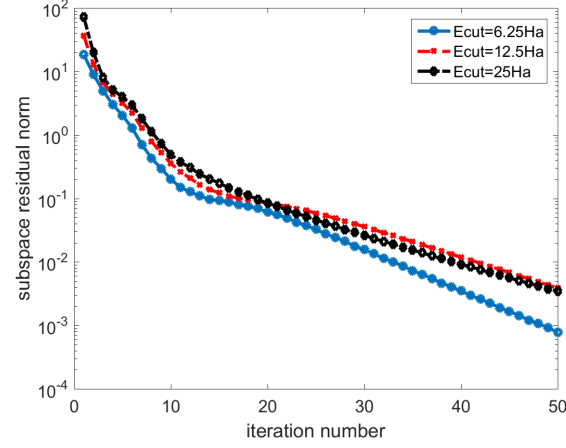


Figure 5: The Convergence of the Davidson algorithm for KS Hamiltonians with different planewave energy cutoff (E_{cut}).

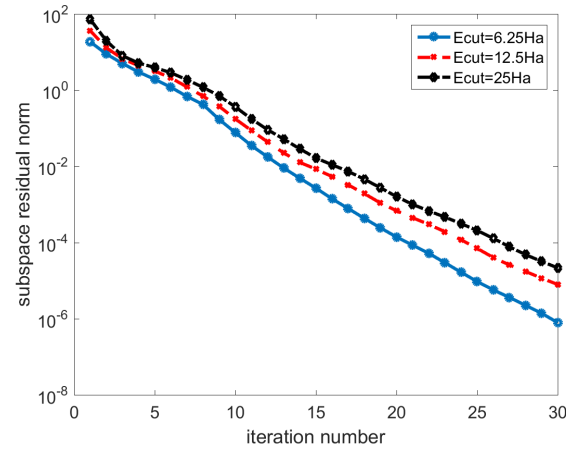


Figure 6: The Convergence of LOBPCG for KS Hamiltonians with different planewave energy cutoff (E_{cut}).

for the use of multigrid preconditioning techniques as well as eliminates the need for FFTs which can lead to better performance and scalability for large problems and distributed computing platforms.

The multigrid preconditioner was developed especially for RMG [Briggs et al., 1996] and the complete description of the discretization is in [Hodak et al., 2007]. There is no theoretical verification for Assumption 1c and 2. The discretization of the Hamiltonian is consistent and stable [Fornberg, 1988], so Assumptions 1a, and 1b, 2b hold. Moreover, the numerical experience with RMG indicates that the all of the Assumptions hold. The RMG preconditioner is a V-cycle for the high-order term (kinetic energy) in the Hamiltonian. There is theory in other contexts [Manteuffel and Parter, 1990] that supports mesh-independence for this kind of preconditioner.

The Laplace operator in the Kohn-Sham Hamiltonian (41) is not diagonal in real-space and is discretized using finite difference operators. In particular, for a regular 3-d grid with orthogonal coordinate axes and a spacing of h between grid points, a discrete Laplacian operator may be defined by

$$\nabla^2 \psi(x_i, y_j, z_k) = c_0 \psi(x_i, y_j, z_k) + \sum_{n=1}^p c_n \left[\psi(x_i \pm nh, y_j, z_k) + \psi(x_i, y_j \pm nh, z_k) + \psi(x_i, y_j, z_k \pm nh) \right], \quad (42)$$

with the triplet (x_i, y_j, z_k) defining the coordinates of each grid point and $x_i = x_0 + ih, y_j = y_0 + jh, z_k = z_0 + kh$. Using this discretization, the Laplacian is not exact but accuracy may be improved by decreasing h and/or increasing p .

We used the RMG electronic structure code to perform the same calculations for a C60 molecule as was done in section 3.3 with a plane wave basis. Instead of using a plane wave cutoff, RMG controls the accuracy of the discretization by varying the grid spacing h , with accuracy increasing as h decreases. The $[0,20] \times [0,20] \times [0,20]$ supercell was represented by cubic grids of 32^3 , 48^3 and 64^3 points. These correspond to grid spacings of $h = 0.625$, $h = 0.417$ and $h = 0.3125$ respectively. The pseudopotential used to model the carbon atoms was again an ONCV [Hamann, 2013] potential but with the non-local terms represented by their values on the real space grid rather than a plane wave expansion in reciprocal space.

RMG uses a multigrid based preconditioner for the Davidson algorithm that treats the current residual $r_i = H\psi_i - \epsilon_i \psi_i$ for a given approximate eigenvector as the right hand side of a Poisson equation.

$$\nabla^2 s_i = H\psi_i - \epsilon_i \psi_i \quad (43)$$

Eq. (43) is then solved using a multigrid poisson solver for the preconditioned residual s_i .

The initial electronic charge density ρ consisted of the sum of the individual atomic charge densities while the initial eigenvectors of the Kohn-Sham Hamiltonian were generated from a linear combination of the 2s and 2p atomic orbitals from each carbon atom. In Fig (7) we plot the convergence with respect to Davidson iteration count for the first SCF step as measured by the Frobenius norm of the residual vectors,

$$\|R\|_F = \|HX - X\Lambda\|_F.$$

In real space X contains the approximate eigenvectors $\{\psi_i(\mathbf{r})\}$, represented by their values on the real space grid while Λ is a diagonal matrix containing the current approximations of the eigenvalues.

The starting estimates from the linear combination of atomic orbitals (LCAO), are closer to the true eigenvectors than the random start used in the plane wave calculation which is reflected in the initially lower eigenspace residual norms.

The RMG convergence rates shown in Fig 7 for h_{grid} 0.312 and 0.417 au are essentially identical, confirming the mesh independence of the Davidson algorithm. There are small differences in convergence rate for the first few iterations, as well as a somewhat different convergence rate for the significantly larger h_{grid} of 0.625 au. The differences are due to weaker convergence criteria automatically applied by the RMG code in the initial Kohn-Sham iterations when solving the Poisson equation, and different round-off errors when representing the Laplacian and the potential on discretized grids with different spacings.

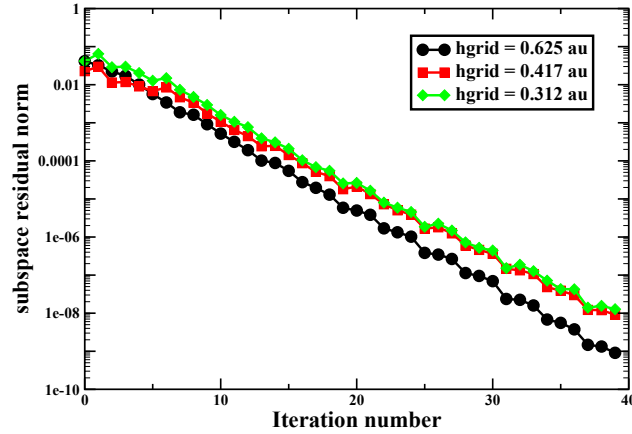


Figure 7: Convergence of the Davidson algorithm in RMG with different mesh sizes (h).

4. Conclusions

In this paper we prove a mesh-independence result for the generalized Davidson algorithm. We report on computations that illustrate the theorem.

5. Data

The programs and input files for the results in § 3 are in the github repository
<https://github.com/ctkelley/DavidsonJCP>

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